CHE 221
Simulation Lab 7

25/03/2025

Fugacity of mixtures

Fugacity of component a in a binary mixture of a and b is given as follows:

$$RT \ln\left[\frac{\hat{f}_a^v}{y_a\, P_{\text{low}}}\right] = -\int_{\frac{n_T\, R\, T}{P_{\text{low}}}}^{V} \left(\frac{\partial P}{\partial n_a}\right)_{V,T,n_b} dV.$$

For the Van der Walls equation of state the integral on the R.H.S can be solved analytically to give

$$\ln\left[\frac{\hat{f}_a^v}{y_a\, P}\right] = \ln[\hat{\phi}_a^v] = -\ln\left[\frac{P\,(v - b_{\text{mix}})}{RT}\right] + \frac{b_a}{v - b_{\text{mix}}} - \frac{2\left(y_a\, a_a + y_b\, \sqrt{a_a\, a_b}\right)}{R\,T\,v}.$$

Here v is the total molar volume, y_a is the mole fraction of a, y_b is the mole fraction of b, b_a is the excluded molar volume of species a, a_a is the a-a interaction, a_b is the b-b interaction, and b_{mix} is the average excluded molar volume parameter. b_{mix} is given by

$$b_{\text{mix}} = \sum_i y_i\, b_i.$$

Use the following values of interaction parameters for this problem:

$$a_a = 0.2\,\text{J}\cdot\text{m}^3\,\text{mol}^{-2},$$
$$a_b = 0.3\,\text{J}\cdot\text{m}^3\,\text{mol}^{-2},$$
$$b_a = 0.00004\,\text{m}^3\,\text{mol}^{-2},$$
$$b_b = 0.00003\,\text{m}^3\,\text{mol}^{-2}.$$

1. Write a MATLAB function that returns the volume of the Van der Walls gas at a fixed P and T. Use the `fzero()` function for this. Note, you will also have to write a residual function and call it from `fzero()` to find v roots of the Van der Walls equation.
2. Plot $\hat{\phi}_a^v$ as a function of pressure (1 -50 bar) for different values of y_a. Use $y_a = 0.2$, 0.5, 0.8, and 1.0.
3. Convert your code to a function and run the `fugacity_slide.m` function to add a slider to your $\hat{\phi}_a^v$ vs. P plot to change the value of a_a dynamically on the plot.
4. Submit a report for all parts by Friday. Late submissions will not be accepted.